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ANFIS pattern for molecular membranes separation optimization

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Research Highlights

- Molecular separation using microporous membranes
- Developing hybrid model based on ANFIS-CFD for the separation
- process Optimization of ANFIS structure for prediction of separation process

Abstract

In this work, molecular separation of aqueous-organic was simulated by using combined soft computing-mechanistic approaches. The considered separation system was a microporous membrane contactor for separation of benzoic acid from water by contacting with an organic phase containing extractor molecules. Indeed, extractive separation is carried out using membrane technology where complex of solute-organic is formed at the interface. The main focus was to develop a simulation methodology for prediction of concentration distribution of solute (benzoic acid) in the feed side of the membrane system, as the removal efficiency of the system is determined by concentration distribution of the solute in the feed channel. The pattern of Adaptive Neuro-Fuzzy Inference System (ANFIS) was optimized by finding the optimum membership function, learning percentage, and a number of rules. The ANFIS was trained using the extracted data from the CFD simulation of the membrane system. The comparisons between the predicted concentration distribution by ANFIS and CFD data revealed that the optimized ANFIS pattern can be used as a predictive tool for simulation of the process. The R^2 of higher than 0.99 was obtained for the optimized ANFIS model. The main privilege of the developed methodology is its very low computational time for simulation of the system and can be used as a rigorous simulation tool for understanding and design of membrane-based systems.

Keywords: Mass transfer; Simulation; Computational models; Separation; Membrane contactors

1. Introduction

Separation using membrane technology has attracted much attention recently due to the unique advantages of this technology compared to other conventional separation and purification technologies [1-6]. The main privilege of membrane separation technology is the high control over separation due to operation in small channel dimensions. Indeed, membrane separation can be conducted at a microscale in which high separation efficiency is attained [7-13]. However, among various membrane operations, membrane contactor (MC) systems have great capability for separation/reaction at a small scale [14-16]. The membrane contactors are commonly porous polymeric membranes used for contacting two liquid or gas phases. The most commonly used module of membrane contactors is hollow-fiber membrane contactor (HFMC) which has found applications in various sectors [17]. These membrane systems provide very high surface area per unit volume and the operation is conducted at microscale [18-21].

In terms of structure, membranes are classified as non-porous and porous in which porous membranes provide better separation performance in terms of mass transfer flux due to the large pore size of membranes [22-30]. However, they do not have a high separation factor in molecular separation. In order to optimize and design membrane contactors for a particular application, modeling of the process can be used as a predictive tool to understand the process and reduce the cost of process development and intensification. Different models can be used for design and optimization of porous membrane contactors in which the main focus is on mass transfer as well as momentum transfer in the module. Computational fluid dynamics (CFD) has been shown great ability in modeling and simulation of mass transfer in different systems [31-33]. For membranes contactors, the modeling is conducted by deriving the governing mass transfer along with momentum transfer equations in all phases of the system [34-36]. The

derived equations are then solved using an appropriate numerical scheme such as finite element or finite volume. Recently, finite element approach has been used extensively for modeling and numerical simulation of mass transfer in hollow-fiber membrane contactors for gas and liquid separation.

The main problem associated with CFD approach in modeling and numerical simulation of mass transfer in porous membrane contactors is the computational expenses which demand high computational time for a numerical solution. Soft computing approach based on fuzzy systems and artificial neural network (ANN) [37-40] have been used recently in modeling and simulation of processes and demand low computational expenses, while great predictive performance has been reported for these approaches [41-43]. However, the accuracy of soft computing methods depends on the architecture of the algorithm used, and the data used for training.

The idea of combining CFD approach and soft computing can be used to capture the advantages of both methods and tackle the drawbacks associated with each method. The method has been recently used for modeling and simulation of multiphase chemical reactors and shown to be a promising approach [41, 42, 44, 45]. This novel approach takes in the data generated by CFD in order to train artificial intelligent system, and once the system has been trained it can be used for prediction of the process without the need for implementation of CFD for the whole system. However, the percentage of data used for training and testing, as well as the structure of the intelligent system play a crucial role in the accuracy of the model. In the current work, a novel simulation methodology is developed by combining CFD and Adaptive Neuro-Fuzzy Inference System (ANFIS) for simulation of porous membrane contactors. The combined model is established by optimization of ANFIS pattern parameters including the percentage of learning

data, type of membership function, and a number of rules. The model is developed and tested for removal of benzoic acid from water in a hollow-fiber membrane contactor.

2. Simulation methodology

2.1. CFD simulation

For CFD simulation of the system, three compartments are considered as the model domains, i.e. feed, membrane, and shell [46, 47]. The feed solution which is aqueous contains benzoic acid (BA) and water, while the organic phase in the shell side includes a complexing agent. By contacting two aqueous and organic phases, a complex of BA-organic is formed and is transferred to the shell side. The BA is removed from the system by convective flow of shell side.

For the CFD simulation of the membrane system, mass and momentum transfer equations are solved. The equations can be represented as follows [20, 48-54]:

$$D\left(\frac{\partial^2 C}{\partial r^2}+\frac{1}{r}\frac{\partial C}{\partial r}+\frac{\partial^2 C}{\partial z^2}\right)=U\frac{\partial C}{\partial z} \tag{1}$$

$$\rho\frac{\partial U}{\partial t}=\nabla\cdot\left[-pI+\mu\left(\nabla U+(\nabla U)^T\right)\right]-\rho(U\cdot\nabla)U+F \qquad \nabla\cdot U=0 \tag{2}$$

where C, D, and U refer to concentration, diffusivity, and velocity of fluid respectively. r and z are the radial and axial coordinates, respectively. The diffusion coefficient of solute is taken from literature [55]. For solving Navier-Stokes equations, finite element method (FEM) was used. FEM was coupled with adaptive meshing and error control using numerical solver of UMFPACK version 4.2.

2.2. ANFIS model

The data generated by CFD simulation of membrane contactor is used to train ANFIS. The data are fed in ANFIS in terms of local concentration distribution at different nodes in the feed channel of HFMC. The local concentration distribution of BA at various nodes are obtained by solution of the mass transfer equation (Eq. 1) coupled with the momentum equation (Eq. 2). The Adaptive-Network-based Fuzzy Inference System (ANFIS) which has an inference fuzzy pattern for simulation of the non-linear behavior of systems was used to predict the concentration distribution of solute [41, 42, 56-58]. Takagi and Sugeno method which is based on *IF-THEN* rule is used for the ANFIS method [59-61]. ANFIS should be trained by a portion of input data, and the trained system is then tested to validate the model. The training data are classified at various levels of membership functions. To find out the optimum pattern of ANFIS for prediction of the process, the ANFIS parameters including the membership function, learning percentage, and a number of rules were changed. The different patterns were compared in terms of R^2 to find out the best fit.

3. Results and discussion

3.1. Effect of *P* factor

P factor which is defined as the percentage of the learning data is the main parameter in the ANFIS model. For this study, the percentage of training data were changed between 2-90 % at three levels, i.e. 0.02, 0.1, and 0.9. The less training data, the faster model, however, the accuracy of testing should be taken into account. The results of comparisons between three different percentages of learning data are illustrated in Fig. 1 for the training data. It is seen that the best fir for the training is obtained for the P factor of 0.02. However, the test data are represented in

Fig. 2 which indicates that the worst fit is obtained when 2 % of data are used for training. When 10 % of CFD data are used for the training of ANFIS, R^2 of 0.98 is obtained, while for 90 % of data, R^2 of 0.99 is observed. It can be seen that 10 % of data would be the optimum *P* factor for the ANFIS, and for the P factors higher than 0.1, no substantial improvement is observed.

The optimum number of *P* factor was then used in order to predict the process. The comparison between CFD and ANFIS results as well as concentration distribution of BA in the feed channel of HFMC is illustrated in Figs. 3 and 4, respectively. It is observed that the predicted concentration distribution by ANFIS matches quite well with the data generated by CFD simulation for the *P* factors of 0.1 and 0.9. Furthermore, the concentration distribution of BA in the membrane contactor (see Fig. 4) indicates that the concentration of BA at the outlet of feed side reaches 0 which implies the efficiency of membrane contactor in the removal of organic compounds from aqueous solutions.

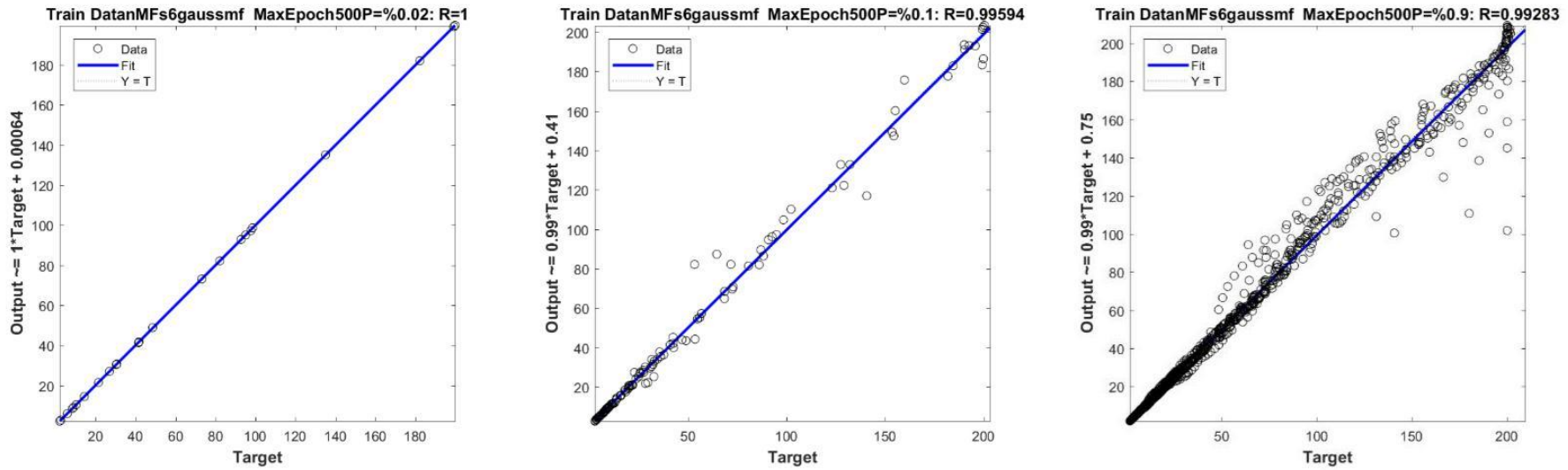


Fig. 1: Comparing CFD with ANFIS results in training stage for different percentage of learning data. Number of rules=6, iterations=500, membership function=gaussmf.

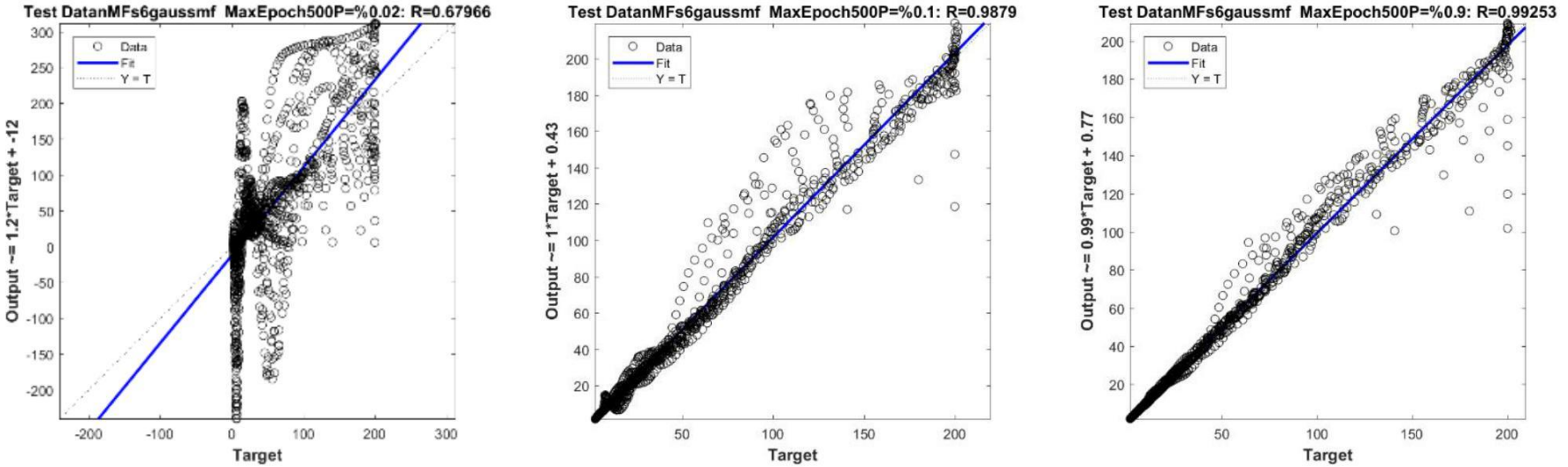


Fig. 2: Comparing CFD with ANFIS results in testing stage for different percentage of learning data. Number of rules=6, iterations=500, membership function=gaussmf.

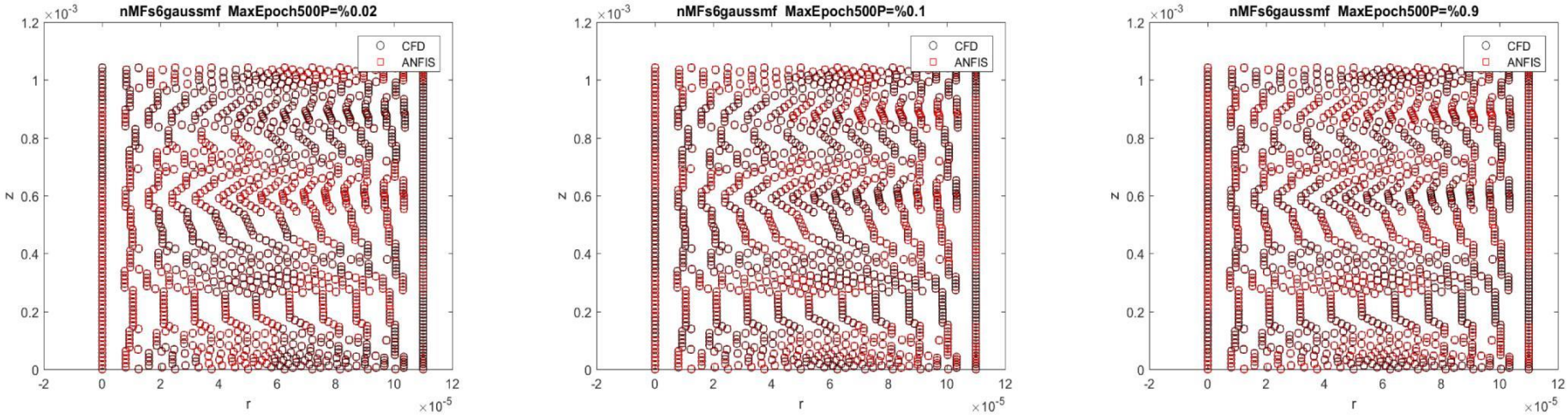


Fig. 3: Comparing CFD with ANFIS results in prediction stage for different percentage of learning data.

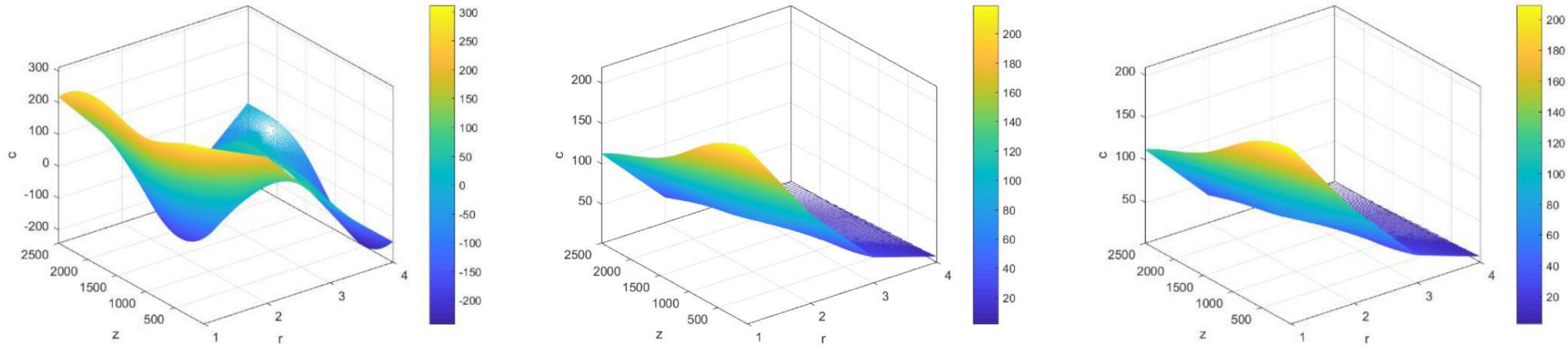


Fig. 4: ANFIS prediction results for different percentage of learning data.

3.2. Effect of membership function

Another ANFIS parameter which was changed in this study is membership functions. To find out the best membership function for simulation of the process, three different membership function including *gauss2mf*, *dsigmf*, and *pimf* were used. These membership functions are the default functions in MATLAB software. The comparisons between various membership functions for the training and testing stages are shown in Figs 5 and 6, respectively. Also, the prediction plots are illustrated in Figs. 7 and 8. The results revealed that the type of membership function does not have a significant effect on the training, testing, and prediction of concentration distribution. Almost, the same R^2 was obtained for all training and testing.

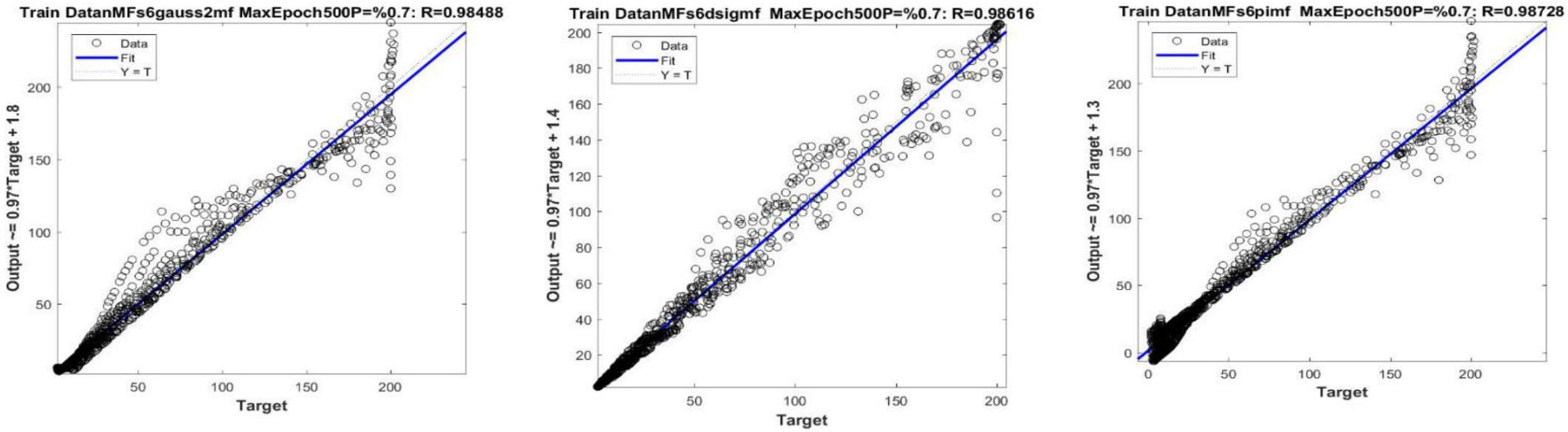


Fig. 5: Comparing CFD with ANFIS results in training stage for different ANFIS membership functions. Number of rules=6, iterations=500, *P*=0.7.

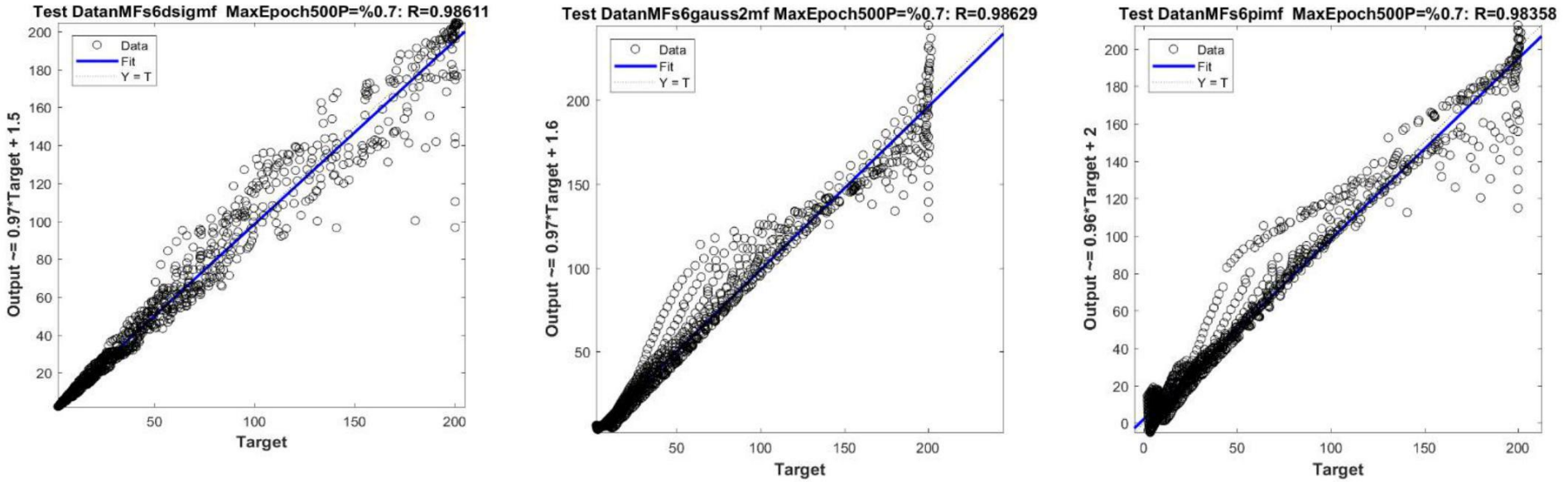


Fig. 6: Comparing CFD with ANFIS results in testing stage for different ANFIS membership functions. Number of rules=6, iterations=500, *P*=0.7.

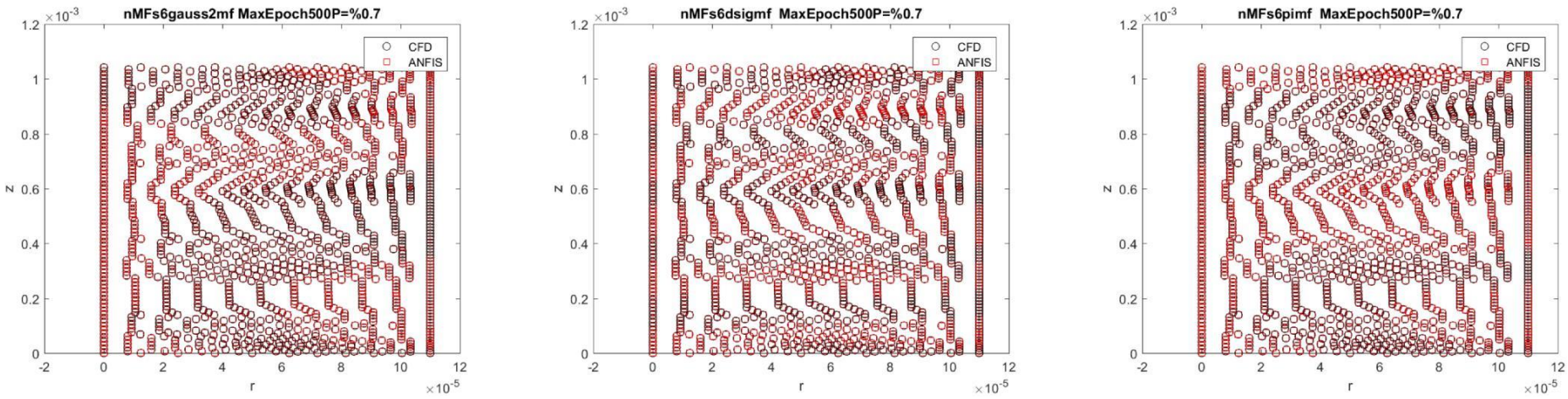


Fig. 7: Comparing CFD with ANFIS results in prediction stage for different ANFIS membership functions.

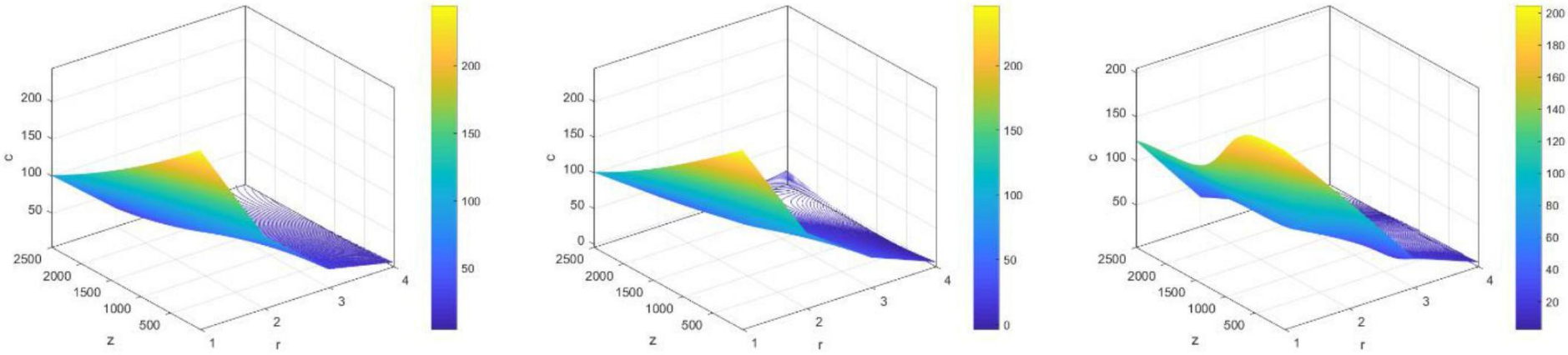


Fig. 8: ANFIS prediction results for different ANFIS membership functions.

3.3. Effect of number of rules

The effect of a number of rules on the accuracy of ANFIS prediction is shown in Figs. 9-11. The fitting for the training and testing are shown in Figs. 9 and 10, respectively, while prediction is shown in Fig. 11. Three number of rules were changed to find out the best pattern for the ANFIS model. 4, 6, and 8 rules were considered in the ANFIS development, while it is seen that the best results are obtained with 6 rules. Increasing the number of rules from 6 to 8 does not improve the fitting significantly, and 6 can be chosen as the optimum number of rules. The concentration distribution of BA in the membrane contactor is depicted in Fig. 11 for a various number of rules. It is seen that the concentration profile cannot be predicted by using 2 rules, whereas the concentration distribution is established by using 6 rules and 8 rules.

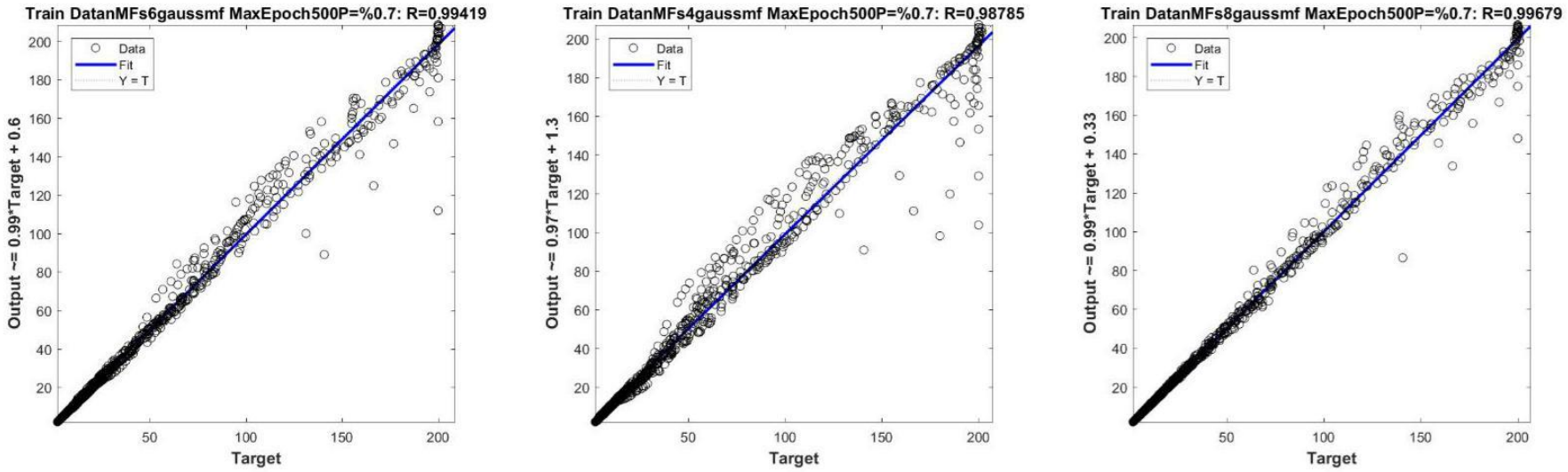


Fig. 9: Comparing CFD with ANFIS results in a training stage for a different number of rules. Membership function=gaussmf, iterations=500, *P*=0.7.

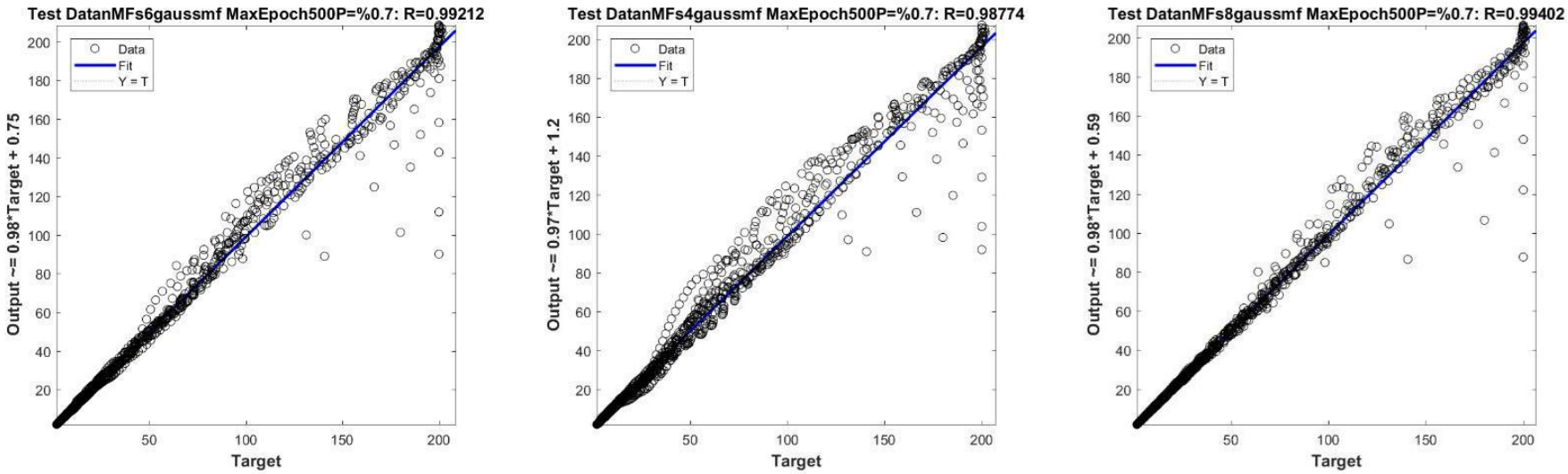
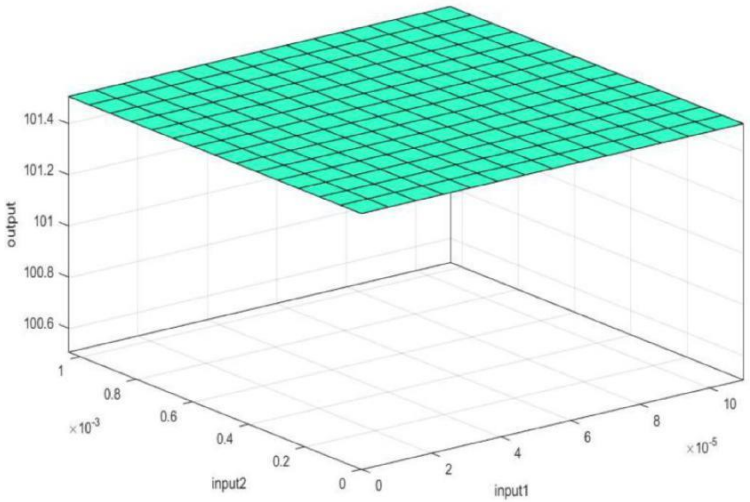
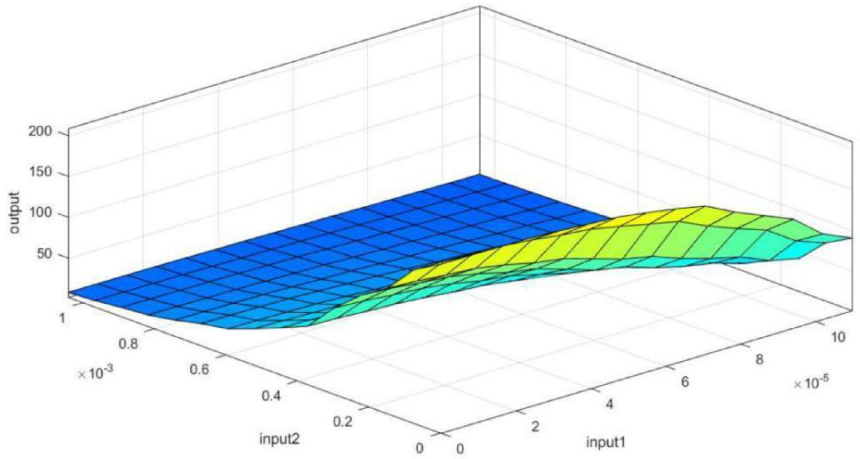


Fig. 10: Comparing CFD with ANFIS results in testing stage for a different number of rules. Membership function=gaussmf, iterations=500, *P*=0.7.

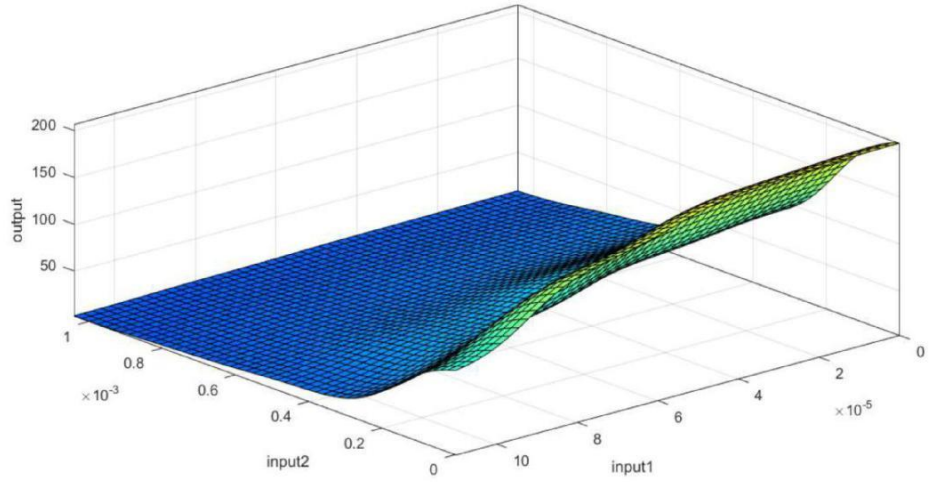
Rule=2



Rule=4



Rule=6



Rule=8

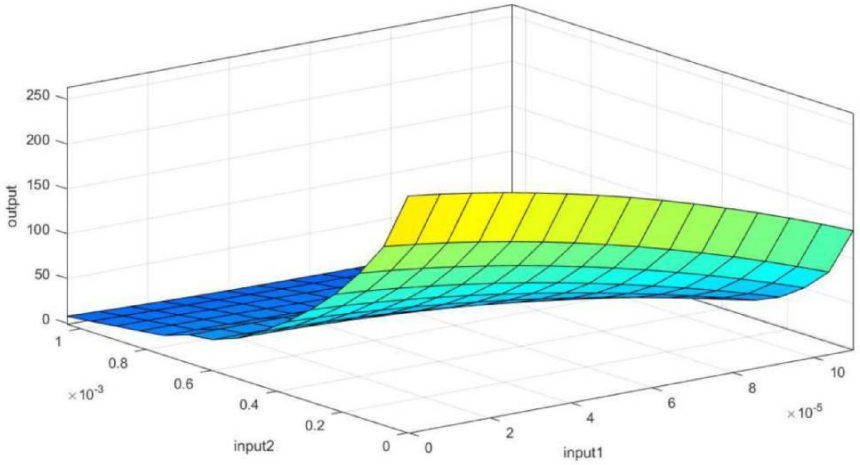


Fig. 11: ANFIS results as a function of and position for a different number of rules.

4. Conclusions

A novel simulation methodology based on CFD-ANFIS was developed in this study to predict the concentration distribution of benzoic acid in a membrane contactor. The CFD data obtained from mass transfer simulation of the process was used in order to train the ANFIS model. The parameters of the ANFIS model were optimized to find the optimum ANFIS pattern for simulation of the process. It was revealed that the optimum ANFIS pattern can be developed using 10 % of learning data, and 6 rules. It was also indicated that the type of membership function does not have a significant effect on the predictability of the model, and almost similar results were obtained for all three considered functions. The results of this novel simulation methodology revealed that this model is robust and powerful in the simulation of membrane separation processes and can be used at low computational expenses compared to other mechanistic models.

Nomenclature

C	[mole m^{-3}]	Concentration of benzoic acid
D	[m^2 s^{-1}]	Diffusion coefficient
F	[N]	Force
p	[Pa]	Pressure
P	[%]	Percentage of learning data
r	[m]	Radial distance
t	[s]	Time
T	[K]	Temperature
U	[m s^{-1}]	Velocity
z	[m]	Axial distance

Greek symbols

η	[kg m^{-1} s^{-1}]	Viscosity
ρ	[kg m^{-3}]	Density

Abbreviations

ANFIS	Adaptive Neuro-Fuzzy Inference System
ANN	Artificial neural network
BA	Benzoic acid
CFD	Computational fluid dynamics
HFMC	Hollow-fiber membrane contactor
MC	Membrane contactor

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